# 2-Iodoethyl isohexanoate

**Inchi:** InChI=1S/C8H15IO2/c1-7(2)3-4-8(10)11-6-5-9/h7H,3-6H2,1-2H3
**InchiKey:** DWAAMYINEBPDQR-UHFFFAOYSA-N
**Formula:** C8H15IO2
**SMILES:** CC(C)CCC(=O)OCCI
**Mol. weight [g/mol]:** 270.11

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -459.48 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 20.15 | kJ/mol | Joback Method |
| hvap | 59.14 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.42 | eV | Cheméo Relay (1.0) |
| log10ws | -2.97 | | Cheméo Relay (1.0) |
| logp | 2.401 | | Crippen Method |
| mcvol | 156.840 | ml/mol | McGowan Method |
| pc | 2619.09 | kPa | Joback Method |
| rinpol | 1313.00 | | NIST Webbook |
| rinpol | 1313.00 | | NIST Webbook |
| tb | 504.41 | K | Cheméo Relay (1.0) |
| tc | 705.44 | K | Cheméo Relay (1.0) |
| tf | 230.16 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 332.76 | J/mol×K | 551.43 | Joback Method |
| cpg | 345.18 | J/mol×K | 586.05 | Joback Method |
| cpg | 356.97 | J/mol×K | 620.67 | Joback Method |
| cpg | 368.15 | J/mol×K | 655.29 | Joback Method |
| cpg | 378.73 | J/mol×K | 689.90 | Joback Method |
| cpg | 388.73 | J/mol×K | 724.52 | Joback Method |
| cpg | 398.16 | J/mol×K | 759.14 | Joback Method |
| dvisc | 0.0044013 | Pa×s | 295.14 | Joback Method |
| dvisc | 0.0020138 | Pa×s | 337.86 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0010982 | Pa×s | 380.57 | Joback Method |
| dvisc | 0.0006768 | Pa×s | 423.29 | Joback Method |
| dvisc | 0.0004559 | Pa×s | 466.00 | Joback Method |
| dvisc | 0.0003281 | Pa×s | 508.72 | Joback Method |
| dvisc | 0.0002485 | Pa×s | 551.43 | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R20049&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point